

## Jan Kuneš

Date of birth: May 27, 1974  
Nationality: Czech Republic  
Office address: Institute of Solid State Physics  
TU Wien  
Wiedner Hauptstr. 8  
1040 Wien  
Austria

### Areas of Research

- Condensed matter theory with focus on real materials
- Electronic correlations and magnetism
- Theory of photoemission, optical and magneto-optical spectroscopies
- Numerical many-body methods
- Density functional methods for solids

### Education

1997 M.Sc. in Physics, Charles University, Prague  
2002 Ph.D. in Physics, Charles University, Prague

### Scientific Career

1998 – 2002 junior research fellow, Institute of Physics ASCR, Czechia  
2002 – 2005 postdoctoral research associate, University of California, Davis, USA  
2006 – 2007 Alexander von Humboldt research fellow, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany  
2007 – 2009 research associate, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany  
2010 – senior staff scientist, Institute of Physics ASCR, Czechia  
2016 – assistant professor, TU Wien, Austria

### Research Visits ( > 1 month)

1999 – 2002 IFW Dresden (12 months)  
2007 University of California, Davis (6 weeks)  
2007, 2010 KITP Santa Barbara (2 month)  
2008 University of Tokyo (1 month)  
2012 École Polytechnique, Paris (1 month)  
2010 – 2015 University of Augsburg (5 months)

## Fellowships, awards and services to the community

2002	Prize of Bolzano Foundation, Charles University, Prague
2002	NATO-NSF Research Fellowship
2006	Alexander von Humboldt Research Fellowship
2008	J. E. Purkyně Fellowship of the Czech Academy of Sciences
2015	APS Outstanding Referee
2015	ERC Consolidator Grant
2016 –	editorial board member Journal of Physics: Condensed Matter

- reviewer for Phys. Rev. B, Phys. Rev. Lett., Adv. Materials, Eur. Phys. Lett., Comput. Phys. Commun., New J. Phys., Science Advances
- grant reviewer for Czech Science Foundation, Dept. of Energy (US), Marsden Fund (New Zealand), TU Wien (Austria), National Science Centre (Poland), Austrian Science Fund, German Research Foundation
- external examiner for M.Sc. degree, K. Dymkowski, Trinity College, Dublin
- member of examination committee for Ph.D. degree, P. Thunström, Uppsala University
- member of the  $\Psi$ -k committee on "Dynamical mean field methods" (since 2012)

## Received grants

2010-2012	<i>Magnetic and transport properties of LaCoO<sub>3</sub>: Dynamical mean-field study</i> , Czech Science Foundation (43.000 EUR)
2010-2012	<i>LDA+DMFT approach to multi-band correlation phenomena: Susceptibilities and structural relaxation</i> , Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), German Research Foundation (280.000 EUR)
2013-2015	<i>Strong electron correlations in systems with spin-orbit coupling</i> , Czech Science Foundation (78.000 EUR)
2013-2015	<i>LDA+DMFT approach to multi-band correlation phenomena</i> , Project P2 of DFG Research Unit 1346 (together with M. Kollar and D. Vollhardt), German Research Foundation (280.000 EUR)
2015-2020	<i>Excitonic Magnetism in Strongly Correlated Materials</i> , ERC Consolidator grant (1.382.000 EUR)

## Teaching

1997	teaching assistant, <i>Practicum in Electricity and Magnetismus</i> , Charles University (1 semester)
2003	lecturer, <i>Magnetism and Magneto-optics in Density Functional Theory</i> , EX-CITING Summer School, Riksgården, Sweden

2011	published lecture notes, <i>Wannier Functions and Construction of Model Hamiltonians</i> , Autumn School 2011: Hands-On Course on LDA+DMFT, Jülich, Germany
2012	lecturer, <i>Wannier Function Projection</i> , Summer School: Bandstructure meets Many Body Theory, Vienna, Austria
2016/WS	Computational Materials Science, TU Wien

## Supervision of students and postdocs

undergraduate student projects:

Karel Pajskr (2015 - 2016)

PhD Students:

Kyo-Hoon Ahn (co-supervising 2013 - )

Dominque Geffroy (co-supervising 2015 - )

Juan Fernandez Afonso (2015 - )

Postdocs:

Vlastimil Křápek (2011-2012)

Pavel Augustinský (2012-2014)

Vladislav Pokorný (2014-2015)

Andrii Sotnikov (2015- )

Atsushi Hariki (2016- )

## Language skills

Czech	native
English	full professional proficiency
German	limited working proficiency

## Scientometry

ResearcherID: B-4484-2008

articles in refereed journals:	77
conference proceedings:	10
book chapters:	2
citations (WoS without self-citations):	~2900
h-index (WoS):	30
invited talks at conferences (seminars):	34 (48)

## List of publications

89. A. Sotnikov and J. Kuneš,  
*Field-induced exciton condensation in LaCoO<sub>3</sub>*  
Sci. Rep. **6**, 30510 (2016).
88. J. Kuneš and D. Geffroy,  
*Spontaneous Spin Textures in Multiorbital Mott Systems*  
Phy. Rev. Lett. **116**, 256403 (2016).
87. P. Wadley, B. Howells, J. Železný, C. Andrews, V. Hills, R. P. Campion, V. Novak, K. Olejnik, F. Maccherozzi, S. S. Dhesi, S. Y. Martin, T. Wagner, J. Wunderlich, F. Freimuth, Y. Mokrousov, J. Kuneš, J. S. Chauhan, M. J. Grzybowski, A. W. Rushforth, K. W. Edmonds, B. L. Gallagher, and T. Jungwirth,  
*Electrical switching of an antiferromagnet*  
Science **351**, 587 (2016).
86. E. Assmann, P. Wissgott, J. Kuneš, A. Toschi, P. Blaha, and K. Held,  
*Woptic: optical conductivity with Wannier functions and adaptive k-mesh refinement*  
Comput. Phys. Commun. **202**, 1 (2016).
85. J. Kuneš,  
*Excitonic condensation in systems of strongly correlated electrons*  
J. Phys.: Condens. Matter **27**, 333201 (2015) - Topical Review
84. J. Panas, A. Kauch, J. Kuneš, D. Vollhardt, and K. Byczuk,  
*Numerical calculation of spectral functions of the Bose-Hubbard model using B-DMFT*  
Phys. Rev. B **92**, 045102 (2015).
83. K.-H. Ahn, K.-W. Lee and J. Kuneš,  
*Doping-dependent bandwidth renormalization and spin-orbit coupling in (Sr<sub>1-x</sub>La<sub>x</sub>)<sub>2</sub>RhO<sub>4</sub>*  
J. Phys.: Condens. Matter **27**, 085602 (2015).
82. J. Kuneš,  
*Phase diagram of exciton condensate in doped two-band Hubbard model*  
Phys. Rev. B **90**, 235140 (2014).
81. J. Kuneš and P. Augustinský,  
*Excitonic condensation of strongly correlated electrons: The case of Pr<sub>0.5</sub>Ca<sub>0.5</sub>CoO<sub>3</sub>.*  
Phys. Rev. B **90**, 235112 (2014).
80. P. Novák, J. Kuneš and K. Knížek,  
*Crystal field of rare earth impurities in LaF<sub>3</sub>*  
Optical Materials **37**, 414 (2014).
79. A. Bauer, A. Regnat, C. G. F. Blum, S. Gottlieb-Schónmeyer, B. Pedersen, M. Meven, S. Wurmehl, J. Kuneš, and C. Pfleiderer,

- Low-temperature properties of single-crystal CrB<sub>2</sub>*  
Phys. Rev. B **90**, 064414 (2014).
78. J. Kuneš and P. Augustinský,  
*Excitonic Instability at the Spin-State Transition in Two-Band Hubbard Model*  
Phys. Rev. B **89**, 115134 (2014).
77. X. Marti, I. Fina, C. Frontera, Jian Liu, P. Wadley, Q. He, R. J. Paull, J. D. Clarkson, J. Kudrnovský, I. Turek, J. Kuneš, D. Yi, J-H. Chu, C. T. Nelson, L. You, E. Arenholz, S. Salahuddin, J. Fontcuberta, T. Jungwirth, and R. Ramesh,  
*Room-temperature antiferromagnetic memory resistor*  
Nat. Mater. **13**, 367 (2014).
76. P. Novák, K. Knížek, M. Maryško, Z. Jiráček, and J. Kuneš,  
*Crystal field and magnetism of Pr<sup>3+</sup> and Nd<sup>3+</sup> ions in orthorhombic perovskites*  
J. Phys.: Condens. Matter **25**, 446001 (2013).
75. M. Brasse, L. Chioncel, J. Kuneš, A. Bauer, A. Regnat, C. G. F. Blum, S. Wurmehl, C. Pfleiderer, M. A. Wilde, and D. Grundler,  
*De Haas-van Alphen effect and Fermi surface properties of single crystal CrB<sub>2</sub>*  
Phys. Rev. B **88**, 155138 (2013).
74. Q. Li, G. Cao, S. Okamoto, J. Yi, W. Lin, B. C. Sales, J. Yan, R. Arita, J. Kuneš, A. V. Kozhevnikov, A. G. Eguiluz, M. Imada, Z. Gai, M. Pan, and D. G. Mandrus,  
*Microscopic and Spectroscopic Evidence for a Slater Metal-Insulator Transition in Sr<sub>2</sub>IrO<sub>4</sub>*  
Sci. Rep. **3**, 3073 (2013).
73. P. Novák, K. Knížek and J. Kuneš,  
*Crystal field parameters with Wannier functions: Application to rare-earth aluminates*  
Phys. Rev. B **87**, 20513 (2013).
72. P. Augustinský, V. Křápek and J. Kuneš,  
*Doping Induced Spin State Transition in LaCoO<sub>3</sub>: Dynamical Mean-Field Study*  
Phys. Rev. Lett. **110**, 267204 (2013).
71. Pavel Augustinský and Jan Kuneš,  
*Improved Green's Function Measurement for Hybridization Expansion Quantum Monte Carlo*  
Comput. Phys. Commun. **184**, 2119 (2013).
70. V. Křápek, P. Novák, J. Kuneš, D. Novoselov, Dm. M. Korotin, and V. I. Anisimov,  
*Spin state transition and covalent bonding in LaCoO<sub>3</sub>*  
Phys. Rev. B **86**, 195104 (2012).
69. P. Wissgott, J. Kuneš, A. Toschi, and K. Held,  
*Dipole matrix element approach vs. Peierls approximation for the optical conductivity*  
Phys. Rev. B **85**, 205133 (2012).

68. J. Kuneš, V. Křápek, N. Parragh, G. Sangiovanni, A. Toschi, and A. V. Kozhevnikov, *Spin state of negative charge-transfer material SrCoO<sub>3</sub>* Phys. Rev. Lett. **109**, 117206 (2012).
67. R. Arita, J. Kuneš, A. V. Kozhevnikov, A. G. Eguiluz, and M. Imada, *Ab initio Studies on the Interplay between Spin-Orbit Interaction and Coulomb Correlation in Sr<sub>2</sub>IrO<sub>4</sub> and Ba<sub>2</sub>IrO<sub>4</sub>* Phys. Rev. Lett. **108**, 086403 (2012).
66. K. Byczuk, J. Kuneš, W. Hofstetter, and D. Vollhardt, *Quantification of correlations in quantum many-particle systems* Phys. Rev. Lett. **108**, 087004 (2012).
65. J. Kuneš, *Wannier functions in The LDA+DMFT approach to strongly correlated materials* in Lecture Notes of the Autumn School 2011 Hands-on LDA+DMFT ed. E. Pavarini, E. Koch, D. Vollhardt, and A. I. Lichtenstein, Forschungszentrum Juelich GmbH Zentralbibliothek, Verlag, 2011
64. J. Kuneš and V. I. Anisimov, *Various scenarios of metal-insulator transition in strongly correlated materials* Ann. Phys. (Berlin) **523**, 682 (2011).
63. J. Kuneš and V. Křápek, *Disproportionation and Metallization at Low-Spin to High-Spin Transition in Multiorbital Mott Systems* Phys. Rev. Lett. **106**, 256401 (2011).
62. J. Kuneš, *Efficient treatment of two-particle vertices in dynamical mean-field theory* Phys. Rev. B **83**, 085102 (2011).
61. J. Kuneš, R. Arita, P. Wissgott, A. Toschi, H. Ikeda, K. Held, *Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions*, Comput. Phys. Commun. **181**, 1888 (2010).
60. J. Kuneš, I. Leonov, M. Kollar, K. Byczuk, V. I. Anisimov, D. Vollhardt, *Dynamical mean-field approach to materials with strong electronic correlations*, Eur. Phys. J. Special Topics **180**, 1 (2010).
59. H. Ikeda, R. Arita and J. Kuneš, *Doping dependence of spin fluctuations and electron correlations in iron pnictides* Phys. Rev. B **82**, 024508 (2010).
58. H. Ikeda, R. Arita and J. Kuneš, *Phase diagram and gap anisotropy in iron-pnictide superconductors*, Phys. Rev. B **81**, 054502 (2010).

57. J. Kuneš, L. Baldassarre, B. Schächner, K. Rabia, C. A. Kuntscher, Dm. M. Korotin, V. I. Anisimov, J. A. McLeod, E. Z. Kurmaev, and A. Moewes, *Metal-insulator transition in  $NiS_{2-x}Se_x$* , Phys. Rev. B **81**, 035112 (2010).
56. M. Sentef, J. Kuneš, P. Werner, and A. P. Kampf, *Correlations in a band insulator*, Phys. Rev. B **80**, 155116 (2009).
55. A. Shitade, H. Katsura, J. Kuneš, X.-L. Qi, S.-C. Zhang, and N. Nagaosa, *Quantum spin Hall effect in a transition metal oxide  $Na_2IrO_3$* , Phys. Rev. Lett. **102**, 256403 (2009).
54. E. R. Ylvisaker, J. Kuneš, A. K. McMahan, and W. E. Pickett, *Charge Fluctuations and the Valence Transition in Yb under Pressure*, Phys. Rev. Lett. **102**, 246401 (2009).
53. J. Kuneš, Dm. M. Korotin, M. A. Korotin, V. I. Anisimov, and P. Werner, *Pressure-Driven Metal-Insulator Transition in Hematite from Dynamical Mean-Field Theory*, Phys. Rev. Lett. **102**, 146402 (2009).
52. V. I. Anisimov, Dm. M. Korotin, S. V. Streltsov, A. V. Kozhevnikov, J. Kuneš, A. O. Shorikov, and M. A. Korotin, *Density-Functional Calculation of the Coulomb Repulsion and Correlation Strength in Superconducting  $LaFeAsO$*  JETP Letters **88**, 729 (2008).
51. V. I. Anisimov, Dm. M. Korotin, M. A. Korotin, A. V. Kozhevnikov, J. Kuneš, A. O. Shorikov, S. L. Skornyakov, and S V. Streltsov, *Coulomb repulsion and correlation strength in  $LaFeAsO$  from Density Functional and Dynamical Mean-Field Theories*, J. Phys.: Condens. Matter **21** 075602 (2009).
50. Jungho Kim, Young-June Kim, J. Kuneš, B. K. Cho, and E. J. Choi, *Optical spectroscopy and electronic band structure of ferromagnetic  $EuB_6$* , Phys. Rev. B **78**, 165120 (2008).
49. J. Kuneš and V. I. Anisimov, *Temperature dependent correlations in covalent insulators: Dynamical mean-field approximation*, Phys. Rev. B **78**, 033109 (2008).
48. F. Tran, J. Kuneš, P. Novák, P. Blaha, L. D. Marks, and K. Schwarz, *Force calculation for orbital-dependent potentials with FP-(L)APW+lo basis set*, Comput. Phys. Commun. **179**, 784 (2008).

47. E. Z. Kurmaev, R. G. Wilks, A. Moewes, L. D. Finkelstein, S. N. Shamin, J. Kuneš, *Oxygen x-ray emission and absorption spectra as a probe of the electronic structure of strongly correlated oxides*, Phys. Rev. B **77**, 165127 (2008).
46. J. Kuneš, A. V. Lukoyanov, V. I. Anisimov, R. T. Scalettar, and W. E. Pickett, *Collapse of magnetic moment drives Mott transition in MnO*, Nat. Mater. **7**, 198 (2008).
45. K.-W. Lee, J. Kuneš, R. T. Scalettar, and W. E. Pickett, *Correlation Effects in the Triangular Lattice Single-band System  $Li_xNbO_2$* , Phys. Rev. B **76**, 144513 (2007).
44. J. Kuneš, V. I. Anisimov, S. L. Skornyakov, A. V. Lukoyanov, and D. Vollhardt, *NiO: Correlated Bandstructure of a Charge-Transfer Insulator*, Phys. Rev. Lett. **99**, 156404 (2007).
43. V. I. Anisimov, A. O. Shorikov, and J. Kuneš, *Magnetic state and electronic structure of plutonium from “first principles” calculations*, J. Alloys Compd. **444-445**, 42 (2007).
42. Deepa Kasinathan, K. Koepnik, J. Kuneš, H. Rosner, W. E. Pickett, *Origin of Strong Coupling in Lithium under Pressure*, Physica C **460-462**, 133 (2007).
41. W. Kuch, F. Offi, L. I. Chelaru, J. Wang, K. Fukumoto, M. Kotsugi, J. Kirschner, and J. Kuneš, *Huge magneto-crystalline anisotropy of x-ray linear dichroism observed on Co/FeMn bilayers*, Phys. Rev. B **75**, 224406 (2007).
40. J. Kuneš, V. I. Anisimov, A. V. Lukoyanov, and D. Vollhardt, *Local correlations and hole doping in NiO: A computational study*, Phys. Rev. B **75**, 165115 (2007).
39. Deepa Kasinathan, J. Kuneš, K. Koepnik, C. V. Diaconu, R. L. Martin, I. Prodan, G. E. Scuseria, N. Spaldin, L. Petit, T. C. Schulthess, and W. E. Pickett, *Mott Transition of MnO under Pressure: Comparison of Correlated Band Theories*, Phys. Rev. B **74**, 195110 (2006).
38. J. Kuneš and W. E. Pickett, *Frustration in the Coupled Rattler System  $KOs_2O_6$* , Phys. Rev. B **74**, 094302 (2006).
37. J. Kuneš and W. E. Pickett, *Effective Hamiltonian for potassium dynamics in the pyrochlore superconductor  $KOs_2O_6$* , phys. stat.sol. (a) **203**, 2962 (2006).



36. P. Schattschneider, S. Rubino, C. Hebert, J. Ruzs, J. Kuneš, P. Novák, E. Carlino, M. Fabrizio, G. Panaccione, and G. Rossi,  
*Detection of magnetic circular dichroism using a transmission electron microscope*,  
Nature **441**, 486 (2006).
35. J. Kuneš and W. E. Pickett,  
*KOs<sub>2</sub>O<sub>6</sub>: superconducting rattler*,  
Physica B: Condensed Matter **378-380**, 898 (2006).
34. P. Novák, J. Kuneš, L. Chaput, and W. E. Pickett,  
*Exact exchange for correlated electrons*,  
phys. stat. sol. (b) **243**, 563 (2006).
33. D. Kashinathan, J. Kuneš, A. Lazicky, H. Rosner, C. S. Yoo, R. T. Scalettar, and W. E. Pickett,  
*Superconductivity and Lattice Instability in Compressed Lithium from Fermi Surface Hot Spots*,  
Phys. Rev. Lett. **96**, 047004 (2006).
32. J. Kuneš, W. Ku, and W. E. Pickett,  
*Exchange Coupling in Eu Monochalcogenides from First Principles*,  
J. Phys. Soc. Japan **74**, 1408 (2005).
31. K.-W. Lee, J. Kuneš, P. Novák, and W. E. Pickett,  
in *New Challenges in Superconductivity: Experimental Advances and Emerging Theories*  
edited by J. Ashkenazi, M.V. Eremin, J. L. Cohn, I. Eremin, D. Manske, D. Pavuna, and  
F. Zuo (Kluwer Academic, Boston, 2004), 235-242
30. J. Kuneš and W. E. Pickett,  
*Exchange coupling in Eu compounds*,  
Physica B: Condensed Matter **359-361**, 205 (2005).
29. K.-W. Lee, J. Kuneš, P. Novák, and W. E. Pickett,  
*Disproportionation, metal-insulator transition, and critical interaction strength in  
Na<sub>1/2</sub>CoO<sub>2</sub>*,  
Phys. Rev. Lett. **94**, 026403 (2005).
28. J. Kuneš, T. Jeong and W. E. Pickett  
*Correlation effects and structural dynamics in the beta-pyrochlore superconductor  
KOs<sub>2</sub>O<sub>6</sub>*,  
Phys. Rev. B **70**, 174510 (2004).
27. J. Kuneš and R. Laskowski,  
*Magnetic ground state and Fermi surface of bcc Eu*,  
Phys. Rev. B **70**, 174415 (2004).

26. K.-W. Lee, J. Kuneš, and W. E. Pickett,  
*Charge disproportionation and spin ordering tendencies in  $\text{Na}_x\text{CoO}_2$ ,*  
Phys. Rev. B **70**, 045104 (2004).
25. J. Kuneš,  
*Magnetism and Magneto-optics in DFT,*  
Physica Scripta **T109**, 166 (2004).
24. J. Kuneš, P. M. Oppeneer, S. Valencia, D. Abramsohn, H.-Ch. Mertins, W. Gudat,  
M. Hecker, C. M. Schneider,  
*Understanding the XMLD and its magnetocrystalline anisotropy at the  $L_{2,3}$ -edges of 3d  
transition metals,*  
J. Magn. Magn. Mater. **272-276**, 2146 (2004).
23. J. Kuneš and W. E. Pickett,  
*Kondo and anti-Kondo coupling to local moments in  $\text{EuB}_6$ ,*  
Phys. Rev. B **69**, 165111(2004).
22. J. Kuneš, H. Rosner, Deepa Kasinathan, C. O. Rodriguez, and W. E. Pickett,  
*heory of orbital moment collapse under pressure in  $\text{FeI}_2$ ,*  
Phys. Rev. B **68**, 115108 (2003).
21. J. Schoenes, R. Repond, F. Hulliger, D. B. Gosh, S. K. De, J. Kuneš, and P. M. Oppeneer,  
*Experimental and theoretical investigation of optical properties of dysprosium monopnic-  
tides,*  
Phys. Rev. B **68**, 085102 (2003).
20. P. Novák, J. Kuneš, W. E. Pickett, Wei Ku, and F. R. Wagner,  
*Self-interaction correction and contact hyperfine field,*  
Phys. Rev. B **67**, 140403(R) (2003).
19. P. M. Oppeneer, H.-Ch. Mertins, D. Abramsohn, A. Gaupp, W. Gudat, J. Kuneš, and C. M.  
Schneider,  
*Buried antiferromagnetic films investigated by x-ray magneto-optical reflection spec-  
troscopy,*  
Phys. Rev. B **67**, 052401 (2003).
18. J. Kuneš and P. M. Oppeneer,  
*Anisotropic x-ray magnetic linear dichroism at the  $L_{2,3}$  edges of cubic Fe, Co, and Ni: Ab  
initio calculations and model theory,*  
Phys. Rev. B **67**, 024431 (2003).
17. J. Kuneš and P. M. Oppeneer,  
*Ab initio calculations of Magneto-optical Effects,*  
Trans. Magn. Soc. Jpn. **2**, 141 (2002).

16. M. Kučera, J. Kuneš, A. Kolomiets, M. Diviš, A. V. Andreev, V. Sechovský, J.-P. Kappler, and A. Rogalev,  
*X-ray magnetic circular dichroism studies of 5f magnetism in UCoAl and UPtAl*,  
Phys. Rev. B **66**, 144405 (2002).
15. J. Kuneš and V. Kamberský,  
*First-principles investigation of the damping of fast magnetization precession in ferromagnetic 3d metals*,  
Phys. Rev. B **65**, 212411 (2002).
14. P. Novák, J. Kuneš, and P. M. Oppeneer,  
*Electronic structure of magnetite*,  
Physica B **312-313**, 785 (2002).
13. J. Kuneš, P. Novák, P. M. Oppeneer, C. König, M. Fraune, U. Rüdiger, G. Güntherodt, and C. Ambrosch-Draxl,  
*Electronic structure of CrO<sub>2</sub> as deduced from its magneto-optical Kerr spectra*,  
Phys. Rev. B **65**, 165105 (2002).
12. J. Kuneš, P. M. Oppeneer, H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, and P. Novák,  
*X-ray Faraday effect of ferromagnetic films: contribution of the core exchange splitting*,  
J. Magn. Magn. Mater. **240**, 454 (2002).
11. J. Kuneš, P. M. Oppeneer, H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, and P. Novák,  
*X-ray Faraday effect at the L<sub>2,3</sub> edges of Fe, Co, and Ni: Theory and experiment*,  
Phys. Rev. B **64**, 174417 (2001).
10. A. V. Andreev, M. Diviš, P. Javorský, K. Prokeš, V. Sechovský, J. Kuneš, and Y. Schiokawa,  
*Electronic structure and magnetism in UPtAl*,  
Phys. Rev. B **64**, 144408 (2001).
9. J. Kuneš, P. Novák, R. Schmid, P. Blaha, and J. Schwarz,  
*Electronic structure of fcc Th: Spin-orbit calculation with 6p<sub>1/2</sub> local orbital extension*,  
Phys. Rev. B **64**, 153102 (2001).
8. H.-Ch. Mertins, F. Schafers, A. Gaupp, W. Gudat, J. Kuneš, and P. M. Oppeneer,  
*Soft X-ray magnetic dichroism and Faraday rotation measured with linearly polarised light*,  
Nucl. Instrum. Meth. A **467&468**, 1407 (2001).
7. H.-Ch. Mertins, P. M. Oppeneer, J. Kuneš, A. Gaupp, D. Abramsohn, and F. Schafers,  
*Observation of the x-ray magneto-optical Voigt effect*,  
Phys. Rev. Lett. **87**, 047401 (2001).
6. J. Kuneš, P. Novák, M. Diviš, and P. M. Oppeneer,  
*Magnetic, magneto-optical, and structural properties of URhAl from first-principles cal-*

- culations,  
Phys. Rev. B **63**, 20511 (2001).
5. K. Krug, K. Winzer, M. Reiffers, J. Kuneš, P. Novák, and F. Kayzel,  
*de Hass-van Alphen effect and the Fermi surface of PrNi<sub>5</sub>*,  
Eur. Phys. J. B **18**, 595 (2000).
  4. J. Kuneš and J. Mistrík,  
*Magnetic, optical and magneto-optical properties of Fe-monolayer from first principles*,  
phys. stat. sol. (b) **220**, 991 (2000).
  3. J. Kuneš and P. M. Oppeneer,  
*Exact many-body sum rule for the magneto-optical spectrum of solids*,  
Phys. Rev. B **61**, 15774 (2000).
  2. J. Kuneš and P. Novák,  
*Full-potential linearized augmented-plane-wave calculation of the magneto-optical Kerr effect in Fe, Co and Ni*,  
J. Phys.: Condens. Matter **11**, 6301 (1999).
  1. M. Kučera, J. Kuneš, and R. Gerber,  
*Magneto-optical effects of Rh<sup>+3</sup> and Rh<sup>+4</sup> doped yttrium iron garnet*,  
J. Appl. Phys. **85**, 5986 (1999).

## Invited presentations

### CONFERENCES

34. Meta-magnetic transition in  $\text{LaCoO}_3$  - a field induced exciton condensation?  
*Computational methods towards engineering novel correlated materials*, Lausanne, Switzerland, October 2016
33. Spin textures in Hubbard systems  
*What about U?*, Trieste, Italy, October 2016
32. Excitonic condensation in models and materials  
*Next generation quantum materials*, Sao Paulo, Brazil, April 2016
31. Excitonic condensation of strongly correlated electrons  
*CORPES 2015*, Paris, France, July 2015
30. Excitonic condensation in systems of strongly correlated electrons  
 *$\Psi$ -k workshop: Strong electron correlation effects in complex d- and f-based magnetic materials for technological applications*, Prague, Czechia, July 2014
29. Excitonic condensation in systems of strongly correlated electrons  
*What about U?*, Lausanne, Switzerland, June 2014
28. Spin-orbit physics of iridates with Wien2k  
*Electronic properties of spin-orbit driven oxides*, Dresden, Germany, September 2013
27. Wannier functions: theory and selected applications  
*Ab initio Dynamical vertex approximation workshop*, Baumschlagerberg, Austria, September 2013
26. Correlation phenomena in the vicinity of spin state transition,  
*Dynamical Mean-Field Approach for Strongly Correlated Materials*, Dresden, Germany, September 2012
25. Thermal and doping effects in materials with competing multiplets,  
*Mini 2012 - workshop on computational condensed matter physics, materials science and nanoscience from first principles*, Barcelona, Spain, January 2012
24. Ordering and Spatial Inhomogeneities in the Vicinity of High-Spin Low-Spin Transitions,  
*Electronic Correlations in Models and Materials*, Augsburg, Germany, September 2011
23. Electronic Correlations in Computer: from Models to Materials,  
*17th Conference of Slovak and Czech Physicists*, Zilina, Slovakia, September 2011
22. Multireference Local States in Solids with Dynamical Mean-Field Theory,  
*Strong Correlations from First Principles*, Seon, Germany, August 2011
21. Dynamical Correlations in Transition Metal Compounds,  
*Goldschmidt 2011*, Prague, Czechia, August 2011

20. Spin State Transitions in Strongly Correlated Systems,  
*The New Generation in Strongly Correlated Electron Systems*, Santiago de Compostela, Spain, July 2011
19. Covalency vs Correlation: Band Insulator with Hubbard U,  
 *$\Psi$ -k 2010*, Berlin, Germany, September 2010
18. Origin of Metal-Insulator Transition in  $\text{NiS}_{2-x}\text{Se}_x$ ,  
*QS2C Theory Forum: 2010 Topical Meeting Advanced First-Principles Calculations and Many-Body Effects in Correlated Electrons*, RIKEN, Tokyo, Japan, September 2010
17. Electronic Correlations in Materials with LDA+DMFT Approach,  
*IUMRS-ICEM 2010*, Seoul, Korea, August 2010
16. From a fluctuating to an intermediate valence: Yb under pressure,  
*Workshop on Recent Developments in Dynamical Mean Field Theory*, Zurich, Switzerland, September 2009
15. Selected Transition Metal Oxides with Dynamical Mean-Field Approximation,  
*Magnetite 2009*, Prague, Czech Republic, January 2009
14. Correlation vs Hybridization in Transition Metal Compounds,  
*Computational Material Science Network Meeting*, Oak Ridge National Laboratory, USA, November 2008
13. Moment Collapse and Metalization in Transition Metal Oxides,  
*16th International Conference on Solid Compounds of Transition Elements*, Dresden, Germany, July 2008
12. Transition Metal Oxides: Mott Transition under Pressure,  
*20th Annual Workshop on Recent Developments in Electronic Structure Methods*, Urbana, IL, June 2008
11. Collapse of Magnetic Moment Drives the Mott Transition in MnO,  
*SFB484 annual meeting*, Irsee, Germany, April 2008
10. Magnetic Moment Collapse-Driven Mott Transition in MnO,  
*March Meeting of American Physical Society*, New Orleans, LA, March 2008
9. Moment-Collapse Driven Mott Transition in MnO under Pressure,  
*Computational Materials Science Network Meeting*, University of California Davis, CA, September 2007
8.  $\text{KOs}_2\text{O}_6$ : Superconducting Rattler,  
*Workshop on Ab Initio Approaches to Electron Phonon Coupling and Superconductivity*, Donostia - San Sebastian, Spain, May 2007

7. NiO - DMFT Study of Charge-Transfer Insulator,  
*Workshop on Realistic Theory of Electron Correlations*, Institute of Physics AS CR,  
Prague, Czech Republic, May 2007
6. Frustration and Lattice Dynamics in Potassium Osmate,  
*M2S-HTSC Conference*, Dresden, Germany, July 2006
5. Charge Disproportionation in  $\text{Na}_{0.5}\text{CoO}_2$  Studied by LDA+U Method,  
*March Meeting of American Physical Society*, Baltimore, MD, March 2006
4. Pyrochlore Superconductors: What is the Difference between K and Rb?,  
*FPLO Workshop*, Leibniz Institute for Solid State Research, Dresden, Germany, March  
2005
3. Ab initio calculations of magneto-optical effects,  
*MORIS 2002*, Benodet, France, May 2002
2. Ab Initio Calculations of Magneto-Optical Kerr Effect,  
*The 6th Prague Colloquium on f-electron Systems*, Prague, Czechia, May 2002
1. Relativistic Local Orbitals in Wien2k: Bulk Properties of Light Actinides,  
*FPLO Workshop*, Leibniz Institute for Solid State Research, Dresden, Germany, March  
2002

## SEMINARS AND COLLOQUIA

48. Excitonic magnetism in models and materials  
University of Fribourg, Switzerland, April 2016
47. Excitonic magnetism in models and materials  
TU Wien, Austria, January 2016
46. Excitonic condensation of strongly correlated electrons  
TU Munich, Germany, December 2015
45. Excitonic condensation of strongly correlated electrons  
European XFEL, Hamburg, Germany, December 2015
44. Excitonic condensation of strongly correlated electrons  
Masaryk University, Brno, Czechia, November 2015
43. Excitonic condensation of strongly correlated electrons  
Technical University of Vienna, Austria, June 2015
42. Excitonic condensation of strongly correlated electrons,  
University of Duisburg, Germany, January 2015
41. Excitonic condensation of strongly correlated electrons,  
Max-Planck Institute for Chemical Physics of Solids, Dresden, November 2014
40. Excitonic condensation in models and materials,  
University of Augsburg, Germany, June 2014
39. Towards material specific theory of ordering phenomena: two-particle response in DMFT,  
Warsaw University, Poland, November 2012
38. Electronic correlations and spin-state transitions,  
Warsaw University, Poland, November 2012
37. Correlation phenomena in the vicinity of spin state transitions,  
Max-Planck Institute for Solid State Research, Stuttgart, Germany, October 2012
36. Electronic correlations in the vicinity of spin state transitions,  
Technical University Dresden, Germany, June 2012
35. Thermal effects in materials with competing multiplets  
Ecole Polytechnique, Paris, France, April 2012
34. Surprising effects of electronic correlations in band insulators, Department of Condensed  
Matter Physics,  
Charles University, Prague, Czechia, October 2011
33. Electronic correlations in computer: from models to materials,  
Masaryk University, Brno, Czechia, October 2011



32. Spin disproportionation at high-spin–low-spin transition in  $\text{LaCoO}_3$ ,  
University of Augsburg, Germany, May 2011
31. Towards material specific theory of ordering phenomena: two-particle response in DMFT,  
University of Wuerzburg, Germany, January 2011
30. Computer simulations of electronic correlations in solids,  
Institute of Physics, Prague, Czechia, October 2010
29. Electronic structure of Strongly Correlated Materials,  
Sungkyunkwan University, Suwon, Korea, August 2010
28. Correlations in Models and Materials,  
Sungkyunkwan University, Suwon, Korea, August 2010
27. Towards Two-Particle Response Functions in DMFT,  
University of Augsburg, Germany, July 2010
26. Electronic Correlations and Covalency: Dynamical Mean-Field Perspective,  
University of Mainz, Germany, June 2010
25. Strongly Correlated Materials with Dynamical Mean-Field Theory,  
Fritz-Haber-Institute, Berlin, Germany, May 2010
24. Electronic Correlations in Models and Materials,  
Theory seminar, Department of Condensed Matter Physics, Charles University, Prague,  
April 2010
23. Electronic Correlation Effects in Solids,  
Department of Condensed Matter Physics, Charles University, Prague, April 2010
22. Correlations & Covalency: Dynamical Mean-Field Theory of Charge-Transfer Com-  
pounds,  
University of California Davis, USA, February 2010
21. From Clusters to Crystals: Application of the Dynamical Mean-Field Theory to Materials,  
CM Theory Department, Institute of Physics, AS CR, Prague, Czechia, February 2010
20. Simultaneous Spin and Metal-Insulator Transition in TM Oxides,  
Ludwig-Maximilians-University Munich, Germany, June 2009
19. What Do the Correlations Do? Selected Materials with Dynamical Mean-Field Theory,  
IFW Dresden, Germany, May 2009
18. Metal-Insulator Transition in  $\text{NiS}_{2-x}\text{Se}_x$ : Is  $\text{NiS}_2$  a Charge-Transfer Insulator?,  
ETH Zurich, Switzerland, February 2009
17. Electronic Structure of  $\text{EuB}_6$ : Insights from Optical Spectroscopy,  
Technical University of Vienna, Austria, January 2009

16. Simultaneous Spin and Metal-Insulator Transition in TM Oxides, University of Tokyo, Japan, November 2008
15. Crystal-Field Driven Mott Transition in MnO under High Pressure, University of Cologne, Germany, May 2008
14. Dynamical Mean-Field Studies of Transition Metal Oxides, Research Center Jülich, Germany, May 2008
13. Mott Transition in MnO under Pressure, Institute of Theoretical Physics, University of Frankfurt, Germany, December 2007
12. The case of two late TMMO's: NiO and MnO investigated by DMFT, Max-Planck-Institute for Solid State Research, Stuttgart, Germany, December 2007
11. Mott Transition in MnO under Pressure: Dynamical Mean-Field Study, University of California Santa Cruz, CA, October 2007
10. Bunsenite - Hole Doping and Local Correlations in Charge Transfer Insulator, Brookhaven National Laboratory, NY, January 2007
9. Hole Doping and Local Correlations in a Charge Transfer Insulator, University of Stony Brook, NY, January 2007
8. Bunsenite - DMFT study of charge-transfer insulator, Ludwig-Maximilian University, Munich, Germany, November 2006
7.  $\text{KOs}_2\text{O}_6$ : a frustrated rattler, Ludwig-Maximilian University, Munich, Germany, June 2006
6.  $\text{KOs}_2\text{O}_6$ : a frustrated rattler, ETH Zurich, Switzerland, February 2006
5.  $\text{KOs}_2\text{O}_6$ : a frustrated rattler, University of Augsburg, Germany, January 2006
4. Lattice dynamics of  $\text{KOs}_2\text{O}_6$ , Oak Ridge National Laboratory, TN, March 2005
3. Exchange coupling in Europium monochalcogenides studied with LDA+U method, University of Augsburg, Germany, January 2005
2. Magnetism of Eu compounds, Max-Planck-Institute for Chemical Physics of Solid State, Dresden, Germany, January 2005
1. Calculation of magneto-optical spectra with LAPW method, Technical University Dresden, Germany, December 1999